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Functions on Adjacent Vertex Degrees of Graphs with Prescribed Degree Sequence*

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Abstract

Zhang et al. [MATCH Commun. Math. Comput. Chem. **78** (2017) 307-322] presented an escalating (de-escalating) function $f(x, y)$ defined on $\mathbb{N} \times \mathbb{N}$, which is a bivariable function such that $f(y, a) + f(x, b) \leq f(x, a) + f(y, b)$ $(f(y, a) + f(x, b) \geq f(x, a) + f(y, b))$ for any $x \geq y$ and $a \geq b$. The connectivity function R_f associated with f is defined as $R_f(G) = \sum\limits_{uv \in E(G)} f(d(u), d(v))$. In this paper, we investigate the properties of the extremal graphs which maximize (minimize) such functions in the set of all simple connected graphs with a given degree sequence. These results are used to characterize the unicyclic graphs which maximize (minimize) such functions among all the unicyclic graphs with a given degree sequence.

1 Introduction

In this paper, we only consider simple connected graphs. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G)$. Let $N(v)$ and $d(v)$ denote the neighbor set and the degree of vertex v, respectively. A nonincreasing sequence of nonnegative integers $\pi = (d_1, d_2, \cdots, d_n)$ is called *graphic degree sequence* if there exists a simple connected graph having π as its vertex degree sequence. Let $\mathcal{G}_\pi$ and $\mathcal{U}_\pi$ denote the general graphs and unicyclic graphs with same degree sequence π, respectively.

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Graph invariants known as topological indices are useful tools for modeling physical and chemical properties of molecules, for design of pharmacologically active compounds, for recognizing environmentally hazardous materials, and so on (see [3], [5] and [6]). In particular, chemical indices play an important role in the research of chemical graph theory (see [1]). Among them, many indices defined on adjacent vertex degrees have been studied extensively. An interesting question in the study of such invariants is to characterize the extremal structures under certain constraints that maximize or minimize a chemical index.

For example, the *Randić index* [2] is probably one of the most well known chemical index, defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-\frac{1}{2}} .$$

Wang [12] characterized the extremal trees with given degree sequence for the Randić index.

The concept of the *Randić index* can be naturally generalized to

$$R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha}$$

for $\alpha \neq 0$, which is called the *connectivity index* (see [2]). The extremal trees for general trees [7], trees with restricted degrees [10] have been characterized in the past years.

The *sum-connectivity index* $W(G)$ [15] and the *general sum-connectivity index* $W_\alpha(G)$ [16] were also introduced as

$$W(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{-\frac{1}{2}}$$

and

$$W_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{\alpha} ,$$

respectively. Many interesting mathematical properties and extremal results on these two indices can be found in [15,16] and the studies that follow. The *third Zagreb index* ([11]), defined as

$$\sum_{uv \in E(G)} (d(u) + d(v))^2 ,$$

is a special case of the general sum-connectivity index with $\alpha = 2$.

Recently, the *Atom-Bond connectivity index* ([4]), defined as

$$\sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} ,$$

has received much attention. Xing and Zhou [14] characterize the extremal trees with fixed degree sequence for atom-bond connectivity index. Lin et al. [8] characterize the extremal graphs with minimal atom-bond connectivity index among all connected graphs with given degree sequence.

In fact, these different but similar invariants can be described by means of a function associated with the degrees of adjacent vertices in a graph. Thus, the extremal structures of graph under certain constraints can be characterized through a unified approach.

Let $f(x, y)$ be a bivariable function defined on $\mathbb{N} \times \mathbb{N}$. $f(x, y)$ is called an escalating function, if $f(y, a) + f(x, b) \leq f(x, a) + f(y, b)$ for any $x \geq y$ and $a \geq b$, with the equality if and only if $x = y$ and $a = b$. Similarly, if $f(y, a) + f(x, b) \geq f(x, a) + f(y, b)$ for any $x \geq y$ and $a \geq b$, with the equality if and only if $x = y$ and $a = b$, $f(x, y)$ is called a de-escalating function (see [13] or [17]).

Definition 1.1 *([13] or [17])The connectivity function R_f associated with f is defined as*

$$R_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)),$$

where $f(x, y)$ is a bivariable function defined on $\mathbb{N} \times \mathbb{N}$.

It is easy to see that $R_f(G)$ describes various chemical indices including the indices mentioned above with different f.

Definition 1.2 *([13]) With given vertex degrees, the greedy tree is achieved through the following greedy algorithm:*

(1) Label the vertex with the largest degree as v (the root);

(2) Label the neighbors of v as $v_1, v_2, \ldots$, assign the largest degrees available to them such that $d(v_{11}) \geq d(v_{12}) \geq \ldots$;

(3) Label the neighbors of v_1 (except v) as v_{11},v_{12},...,such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \ldots$, then do the same for $v_2, v_3, \ldots$;

(4) Repeat (3) for all the newly labeled vertices. Always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

In [13, 17], the following is shown.

Theorem 1.3 *([13]or [17]) For any escalating function f, R_f is maximized by the greedy tree among trees with given degree sequence.*

Theorem 1.4 *([13]or [17]) For any de-escalating function f, R_f is minimized by the greedy tree among trees with given degree sequence.*

Recently, Zhang et al. in [17] compare the extremal trees of different degree sequences. A nonincreasing sequence of nonnegative integers π is called *a unicyclic degree sequence* if there exists a unicyclic graph having π as its vertex degree sequence. Motivated by the above results, we will characterize the extremal unicyclic graphs which maximize or minimize R_f in $\mathcal{U}_\pi$.

Theorem 1.5 *Given a unicyclic degree sequence π, R_f is maximized by U_π^* (defined in Section 3) for any escalating function f and minimized by U_π^* for any de-escalating function f in $\mathcal{U}_\pi$.*

The rest of this paper is organized as follows: In section 2, the properties of the extremal graphs which maximize R_f associated with an escalating function f in $\mathcal{G}_\pi$ are studied. In section 3, the extremal graphs which maximize R_f associated with an escalating function f in $\mathcal{U}_\pi$ are characterized. In section 4, the extremal graphs which minimize R_f associated with a de-escalating function f in $\mathcal{U}_\pi$ are characterized. In section 5, some examples of the application of our findings to specific graph invariants are presented.

2 The extremal graphs in $\mathcal{G}_\pi$ for escalating function

Let $G-uv$ denote the graph obtained from G by deleting an edge uv in G and $G+uv$ denote the graph obtained from G by adding an edge uv. The following lemmas will be used in our proof.

Lemma 2.1 *Assume that f is an escalating function. Let $G \in \mathcal{G}_\pi$ with $uv, xy \in E(G)$ and $uy, vx \notin E(G)$. Let $G' = G-uv-xy+uy+xv$. If $d(u) \geq d(x)$ and $d(y) \geq d(v)$, then $R_f(G) \leq R_f(G')$. Moreover, $R_f(G) < R_f(G')$ if and only if both inequalities are strict.*

Proof. From definition 1.1,

$$\begin{aligned} R_f(G) - R_f(G') &= \sum_{st\in E(G)} f(d(s),d(t)) - \sum_{st\in E(G')} f(d(s),d(t)) \\ &= f(d(u),d(v)) + f(d(x),d(y)) - f(d(u),d(y)) - f(d(x),d(v)) \\ &\leq 0. \end{aligned}$$

So $R_f(G) \leq R_f(G')$. Moreover, $R_f(G) < R_f(G')$ if and only if both inequalities are strict.

■

Theorem 2.2 *For any escalating function f, there exists an extremal graph G which maximizes R_f in $\mathcal{G}_\pi$ such that the vertices of G can be relabeled as $\{v_1, v_2, \cdots, v_n\}$ such that the following hold:*

(1) $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v)$ is the distance between vertex v and root v_1;

(2) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$;

(3) Suppose v_iv_j, $v_sv_t \in E(G)$ and v_iv_t, $v_sv_j \notin E(G)$ with $h(v_j) = h(v_t) = h(v_i) + 1 = h(v_s) + 1$. If $i < s$, then $j < t$.

Proof. Let H be an extremal graph which maximizes R_f in $\mathcal{G}_\pi$. Then the vertices of H can be relabeled as $V(H) = \{v_1, v_2, \cdots, v_n\}$ such that $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$ and $p < q$ if $d(v_p) > d(v_q)$ and $h(v_p) = h(v_q)$, where $d(v_1)$ is the maximum degree of H. In the following, we will construct an extremal graph $G \in \mathcal{G}_\pi$ which maximizes R_f in $\mathcal{G}_\pi$ from H such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$.

If the condition (2) does not hold for H, there exists the smallest integer i in $\{1, 2, \cdots, n\}$ such that there is another integer j such that $i < j$ and $d(v_i) < d(v_j)$. Choose j such that $d(v_j) \geq d(v_s)$ for all $s \geq j + 1$. It is easy to see that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_{i-1}) \geq d(v_k)$ for all $i \leq k \leq n$. Since $d(v_1)$ is the maximum degree of H, we have $i \geq 2$ and $h(v_j) \geq h(v_i) \geq 1$. Assume $h(v_i) = h(v_j)$. Since $p < q$ if $d(v_p) > d(v_q)$ and $h(v_p) = h(v_q)$, we have $j < i$, a contradiction. So we have $h(v_i) < h(v_j)$.

Let $u_iv_i \in E(H)$ such that $h(v_i) = h(u_i) + 1$. Clearly, $u_i \in \{v_1, v_2, \cdots, v_{i-1}\}$ and $h(v_j) > h(v_i) \geq 1$. Note that $i < j$ and $d(v_i) < d(v_j)$. There is a vertex $u_j \in N(v_j)$ such that $u_i \neq u_j$ and $u_iv_j, u_jv_i \notin E(H)$. Clearly, $d(u_i) \geq d(u_j)$ if $u_j \in \{v_{i+1}, v_{i+2}, \cdots, v_n\}$. If $u_j \in \{v_1, v_2, \cdots, v_{i-1}\}$, we also have $d(u_i) \geq d(u_j)$, since $h(u_i) < h(v_i) \leq h(u_j)$. Let $G_1 = H - u_iv_i - u_jv_j + u_iv_j + u_jv_i$. Then we have $G_1 \in \mathcal{G}_\pi$ such that $R_f(H) \leq R_f(G_1)$ by Lemma 2.1. Let $w_i = v_j$, $w_j = v_i$ and $w_k = v_k$ for $k \neq i, j$. Then G_1 is an extremal graph which maximizes R_f in $\mathcal{G}_\pi$ such that the vertices of G_1 can be relabeled as $V(G_1) = \{w_1, w_2, \cdots, w_n\}$ such that $h(w_1) \leq h(w_2) \leq \cdots \leq h(w_n)$, $d(w_1) \geq d(w_2) \geq \cdots \geq d(w_i) \geq d(w_k)$ for all $k \geq i + 1$, and $p < q$ if $d(w_p) > d(w_q)$ and $h(w_p) = h(w_q)$. If the condition (2) does not hold for G_1, we can repeat the above process, and finally get an extremal graph G which maximizes R_f in $\mathcal{G}_\pi$ such that (1) and (2) hold.

Further, if there are four vertices satisfying v_iv_j, $v_sv_t \in E(G)$ and v_iv_t, $v_sv_j \notin E(G)$ with $h(v_j) = h(v_t) = h(v_i) + 1 = h(v_s) + 1$ and $i < s$, then $j < t$. Otherwise, without loss of generality, assume that $d(v_t) > d(v_j)$. Let $G_2 = G - v_iv_j - v_sv_t + v_iv_t + v_sv_j$. Since $d(v_i) \geq d(v_j)$ and $d(v_t) > d(v_s)$, we have $G_2 \in \mathcal{G}_\pi$ with $R_f(G) \leq R_f(G_2)$ by Lemma 2.1. Repeat the above process, we can construct the new extremal graph which maximizes R_f from G such that the above three conditions (1), (2) and (3) hold. The proof is completed.

■

3 The extremal graphs in $\mathcal{U}_\pi$ for escalating function

Let $\pi = (d_1, d_2, \cdots, d_n)$ be a unicyclic graphic degree sequence such that $d_n = 2$. Clearly, the cycle is the only graph having degree sequence π. So in the following we always suppose $d_n = 1$.

Lemma 3.1 *For any escalating function f, there exists an extremal graph G which maximizes R_f in $\mathcal{U}_\pi$ such that $v_1v_2, v_1v_3, v_2v_3 \in E(G)$, where v_1, v_2 and v_3 are three vertices such that $d(v_1) \geq d(v_2) \geq d(v_3) \geq d(x)$ for all $x \in V(G) \setminus \{v_1, v_2, v_3\}$.*

Proof. By Theorem 2.2, there is an extremal graph G which maximizes R_f in $\mathcal{U}_\pi$ such that the vertices of G can be relabeled as $\{v_1, v_2, \cdots, v_n\}$ such that the following hold:

(1) $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v)$ is the distance between vertex v and root v_1;

(2) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$;

(3) Suppose v_iv_j, $v_sv_t \in E(G)$ and v_iv_t, $v_sv_j \notin E(G)$ with $h(v_j) = h(v_t) = h(v_i) + 1 = h(v_s) + 1$. If $i < s$, then $j < t$.

Let $h(G) = \max\limits_{v \in V(G)} h(v)$ and $W_i = \{v \in V(G) | h(v) = i\}$ with $|W_i| = n_i$ for $0 \leq i \leq h(G)$. It is easy to see that $W_0 = \{v_1\}$ and $n_1 = d(v_1)$. In the following, we relabel the vertices of G. Let $v_1 = v_{01}$. The vertices in W_1 are relabeled as $v_{11}, v_{12}, \cdots, v_{1,n_1}$ such that $d(v_{11}) \geq d(v_{12}) \geq \cdots \geq d(v_{1,n_1})$, where $v_{11} = v_1$ and $v_{12} = v_2$. Assume that the vertices in W_t have been already relabeled as $v_{t1}, v_{t2}, \cdots, v_{t,n_t}$. Then the vertices in W_{t+1} can be relabeled as $v_{t+1,1}, v_{t+1,2}, \cdots, v_{t+1,n_{t+1}}$ such that they satisfy the following conditions: if $v_{tk}v_{t+1,i}$, $v_{tk}v_{t+1,j} \in E(G)$ with $i < j$, then $d(v_{t+1,i}) \geq d(v_{t+1,j})$; if $v_{tk}v_{t+1,i}, v_{tl}v_{t+1,j} \in E(G)$ with $k < l$, then $i < j$. Let C_G be the only cycle of G. We consider two cases:

Case 1: $d_2 = 2$. Then $d(v_{01}) = d_1 \geq 3$. Clearly, $v_{01} \in V(C_G)$.

If there are two vertices v_{1i}, v_{1j} with $v_{1i}v_{1j} \in E(G)$ with $1 \leq i < j \leq n_1$, then $d(v_{1i}) = d(v_{1j}) = 2$. The assertion holds.

If $v_{1i}v_{1j} \notin E(G)$ for any $1 \leq i < j \leq n_1$, there are three vertices $v_{1s}, v_{1t} \in V(C_G)$ and $v_{1r} \notin V(C_G)$. It is easy to see that $d(v_{1s}) = d(v_{1t}) = d(v_{1r}) = 2$. Then there are two vertices $v_{2k} \in V(C_G)$ and $v_{2m} \notin V(C_G)$ such that $v_{1s}v_{2k} \in E(C_G)$ and $v_{1r}v_{2m} \in E(G)$. Let $G_1 = G - v_{1s}v_{2k} - v_{1r}v_{2m} + v_{1s}v_{1r} + v_{2k}v_{2m}$. Then $G_1 \in \mathcal{U}_\pi$ with $R_f(G) \leq R_f(G_1)$ by Lemma 2.1. The assertion holds.

Case 2: $d_2 \geq 3$. If $v_{11}v_{12} \in E(G)$, the assertion holds. In the following, we assume $v_{11}v_{12} \notin E(G)$.

Claim1: There is an extremal graph H which maximizes R_f in $\mathcal{U}_\pi$ with the only cycle C_H such that $v_{01} \in V(C_H)$ and $v_{01}v_{11}, v_{01}v_{12} \in E(H)$.

Assume the Claim 1 does not hold for all extremal graphs which maximize R_f in $\mathcal{U}_\pi$. Note that there is a path $P = ux_1x_2\cdots x_tv_{01}v_{1t}y_1y_2\cdots y_m$ such that v_{01} is on the path P, where $u \in V(C_G)$,$x_1 \notin V(C_G)$ and $d(y_m) = 1$. Choose $xy \in E(C_G)$ with $x \neq u$,$y \neq u$ and $\min\{h(x), h(y)\} \geq 2$. It is easy to see that $d(v_{1t}) \geq max\{d(x), d(y)\}$. If $d(x) \leq d(y_{m-1})$, let $H = G - xy - y_{m-1}y_m + xy_m + yy_{m-1}$. Then $H \in \mathcal{U}_\pi$ with $R_f(G) \leq R_f(H)$ by Lemma 2.1 and $v_{01} \in V(C_H)$, a contradiction. If $d(y) \leq d(y_{m-1})$, let $H = G - xy - y_{m-1}y_m + yy_m + xy_{m-1}$. Then $H \in \mathcal{U}_\pi$ with $R_f(G) \leq R_f(H)$ by Lemma 2.1 and $v_{01} \in V(C_H)$, a contradiction. So we have $\min\{d(x), d(y)\} > d(y_{m-1})$. Similarly, we have $\min\{d(x), d(y)\} > d(y_{m-2})$. Repeating the above process, we have $\min\{d(x), d(y)\} > d(v_{1t})$, a contradiction. So the Claim 1 holds.

Claim 2: There is an extremal graph H which maximizes R_f in $\mathcal{U}_\pi$ with the only cycle C_H such that $v_{01}v_{11} \in E(C_H)$ and $v_{01}v_{12} \in E(H)$.

Assume the Claim 2 does not hold for any extremal graph H which maximizes R_f such that $v_{01} \in V(C_H)$ and $v_{01}v_{11}, v_{01}v_{12} \in E(H)$ in $\mathcal{U}_\pi$. If $v_{11} \notin V(C_H)$, there is a path $P = v_{01}v_{11}w_1w_2\cdots w_s$ with $w_1 \notin V(C_H)$ and $d(w_s) = 1$. Choose $xy \in E(C_H)$ with $x \neq v_{01}$ and $y \neq v_{01}$. Clearly, $d(v_{11}) \geq max\{d(x), d(y)\}$. The Claim 2 holds by the similar proof with Claim 1.

Claim 3: There is an extremal graph H which maximizes R_f in $\mathcal{U}_\pi$ with the only cycle C_H such that $v_{01}v_{11}, v_{01}v_{12} \in E(C_H)$.

There exists an extremal graph G with $v_{01}v_{11} \in E(C_G)$ and $v_{01}v_{12} \in E(G)$ by Claim 2. If $v_{01}v_{12} \notin E(C_G)$, then $v_{12} \notin V(C_G)$ such that there is a vertex $y \neq v_{01}$ with $v_{12}y \in E(G)$. There is also a vertices $x \neq v_{01}$ such that $v_{11}x \in E(C_G)$. Clearly, $d(v_{12}) \geq d(x)$ and

$d(v_{11}) \geq d(y)$. Let $H = G - v_{11}x - v_{12}y + v_{11}v_{12} + xy$. Then $H \in \mathcal{U}_\pi$ such that $v_{12} \in V(C_H)$ and $R_f(G) \leq R_f(H)$ by Lemma 2.1.

Claim 4: There is an extremal graph H which maximizes R_f in $\mathcal{U}_\pi$ with the only cycle C_H such that $V(C_H) = \{v_{01}, v_{11}, v_{12}\}$.

There is an extremal graph G which maximizes R_f in $\mathcal{U}_\pi$ with the only cycle C_G such that $v_{01}v_{11}, v_{01}v_{12} \in E(C_G)$ by Claim 3. Note that $d(v_{11}) \geq 3$. There are two vertices $x \notin V(C_G)$ and $y \in V(C_G)$ such that $x \neq v_{01}$, $v_{11}x \in E(G)$ and $v_{12}y \in E(C_G)$. Let $H = G - v_{11}x - v_{12}y + v_{11}v_{12} + xy$. Then $H \in \mathcal{U}_\pi$ with $R_f(G) \leq R_f(H)$ by Lemma 2.1. The proof is completed. ■

Let $\pi = (d_1, d_2, \cdots, d_n)$ be a unicyclic graphic degree sequence such that $d_1 \geq d_2 \geq \cdots \geq d_n$. We now construct a unicyclic graph as follows. Select a vertex v_{01} as a root and begin with v_{01} of the zero-th layer. Let $s_1 = d_1$ and select s_1 vertices $v_{11}, v_{12}, \cdots, v_{1s_1}$ of the first layer such that they are adjacent to v_{01}, and v_{11} is adjacent to v_{12}. In general, assume that all vertices of the t-st layer have been constructed and are denoted by $v_{t1}, v_{t2}, \cdots, v_{t,s_t}$. We construct all the vertices of the $(t+1)$-st layer by the induction hypothesis. Let $s_{t+1} = d_{s_1+\cdots+s_{t-1}+2} + \cdots + d_{s_1+\cdots+s_t+2} - s_t$ and select s_{t+1} vertices $v_{t+1,1}, v_{t+1,2}, \cdots, v_{t+1,s_{t+1}}$ of the$(t+1)$st layer such that v_{t1} is adjacent to $v_{t+1,1}, \cdots, v_{t+1,d_{s_1+\cdots+s_{t-1}+1}-1}$, $\cdots$, v_{t,s_t} is adjacent to $v_{t+1,s_{t+1}-d_{s_1+\cdots+s_t}+2}, \cdots, v_{t+1,s_{t+1}}$. Then we get a unicyclic graph $U^*_{\pi,}$ with degree sequence π (see Fig.1 for an example).

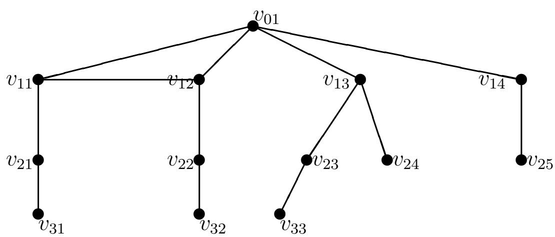

Figure 1 $\quad U^*_\pi$ with $\pi = (4, 3, 3, 3, 2, 2, 2, 2, 1, 1, 1, 1, 1)$

Theorem 3.2 *For any escalating function f, R_f is maximized by U^*_π in $\mathcal{U}_\pi$.*

Proof. By Lemma 3.1, there exists an extremal graph H which maximizes R_f in $\mathcal{U}_\pi$ such that $v_1v_2, v_1v_3, v_2v_3 \in E(H)$, where v_1, v_2 and v_3 are three vertices such that $d(v_1) \geq d(v_2) \geq d(v_3) \geq d(x)$ for all $x \in V(G) \setminus \{v_1, v_2, v_3\}$. By similar proof with Theorem 2.2, there exists an extremal graph G which maximizes R_f in $\mathcal{U}_\pi$ such that the vertices of G can be relabeled as $\{v_1, v_2, \cdots, v_n\}$ such that the following hold:

(1) $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v)$ is the distance between vertex v and root v_1;

(2) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$;

(3) Suppose v_iv_j, $v_sv_t \in E(G)$ and v_iv_t, $v_sv_j \notin E(G)$ with $h(v_j) = h(v_t) = h(v_i) + 1 = h(v_s) + 1$. If $i < s$, then $j < t$.

(4) v_1v_2, v_1v_3,$v_2v_3 \in E(G)$.

Clearly, G must be U^*_π. The proof is completed. ■

4 The extremal graphs in $\mathcal{U}_\pi$ for de-escalating function

We can get the corresponding results for de-escalating function by similar techniques as above.

Theorem 4.1 *For any de-escalating function f , there is an extremal graph G which minimizes R_f in $\mathcal{G}_\pi$ such that the vertices of G can be relabeled as $\{v_1, v_2, \cdots, v_n\}$ such that the following hold:*

(1) $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v)$ is the distance between vertex v and root v_1;

(2) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$;

(3) Suppose v_iv_j, $v_sv_t \in E(G)$ and v_iv_t, $v_sv_j \notin E(G)$ with $h(v_j) = h(v_t) = h(v_i) + 1 = h(v_s) + 1$. If $i < s$, then $j < t$.

Theorem 4.2 *For any de-escalating function f, R_f is minimized by U^*_π in $\mathcal{U}_\pi$.*

Clearly, Theorem 1.5 follows from Theorem 3.2 and 4.2.

5 Applications

In this section we present the application of our results to specific graph invari- ants.

Lemma 5.1 *([17]) The bivariable function $f(x, y) = (x + y)^\alpha$, defined on $\mathbb{N} \times \mathbb{N}$, is escalating for $\alpha \geq 1$ and de-escalating for $0 < \alpha < 1$.*

Lemma 5.2 *([17]) The bivariable function $f(x, y) = x^\alpha y^\alpha$, defined on $\mathbb{N} \times \mathbb{N}$, is an escalating (de-escalating) function for $\alpha > 0$ ($\alpha < 0$).*

Lemma 5.3 *([17]) The bivariable function* $f(x,y) = \sqrt{\frac{x+y-2}{xy}}$*, defined on* $\mathbb{N} \times \mathbb{N}$*, is a de-escalating function.*

By Theorem 3.2 and 4.2, we get the following results.

Corollary 5.4 *Given a unicyclic degree sequence* π*,* U_π^* *has the maximum general sum-connectivity index for* $\alpha \geq 1$ *and connectivity index for* $\alpha > 0$ *in* $\mathcal{U}_\pi$*, respectively.*

Corollary 5.5 *Given a unicyclic degree sequence* π*,* U_π^* *has the minimum Randić index, general sum-connectivity index for* $0 < \alpha < 1$*, connectivity index for* $\alpha < 0$*, and the Atom- Bond connectivity in* $\mathcal{U}_\pi$*, respectively.*

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